BJRS
BRAZILIAN JOURNAL OF RADIATION SCIENCES

doi.org/10.15392/2319-0612.2024.2425
2024, 12(3) | 01-15 | e2425
Submitted: 2024-01-24
Accepted: 2024-07-01

Multiphysics Computational Modeling of Nuclear Reactors Small Size Through the Coupling of Serpent Codes and Fluent

Lago [a*], E. S.; Dominguez, D. S.[a**]; Mazaíra, L. R [b***]

[a] State University of Santa Cruz, 45662-900, Ilhéus, Bahia, Brazil.
[b] Federal University of Pernambuco, 50670-901, Recife, Pernambuco, Brazil

Correspondence: *eng.eriklago@gmail.com **dsdominguez@uesc.br ***leored1984@gmail.com

Abstract: The study of nuclear energy using computational codes has been widely explored by nuclear engineering researchers through various calculations over the years, with emphasis on neutron and thermo-hydraulic calculations. The need for designing a reactor model that would produce energy at a lower cost per MWh highlighted the importance of Small Modular Reactor (SMR) reactors. **Development:** The present work aims to carry out a study related to the coupling of two computational codes, SERPENT and ANSYS FLUENT, using an SMR PWR reactor model (Pressurized Water Reactor) from the company B&W Generation, called mPower. **Methods:** The geometry of a pin of the mPower reactor was modeled and neutronics analyses of the model were performed using SERPENT code, while thermo-hydraulic analysis was simulated using FLUENT code. A coupling algorithm between these two simulation tools was built to automate the process of obtaining operational conditions for the effective operation of the reactor. **Results:** This work enabled the development of a tool that performs the multiphysics coupling between neutronic and thermos-hydraulic phenomena on mPower fuel pin. **Conclusion:** Multiphysics simulation, which considers the interaction between neutronic and thermal dynamics, provides an enhanced understanding of reactor operation. In this simulation, the power distribution generated by the neutronic code is used as input for the thermo-hydraulic code. Conversely, the temperature distribution obtained from the thermo-hydraulic simulation is fed back into a subsequent iteration of the neutronic analysis, thus achieving a coupling between these phenomena. To obtain accurate estimates for the power and temperature distributions, an automated process based on Python programming was implemented.

Keywords: SERPENT, FLUENT, mPower, nuclear reactors, multiphysics coupling, computational modeling.

BJRS
BRAZILIAN JOURNAL OF RADIATION SCIENCES

doi.org/10.15392/2319-0612.2024.2425
2024, 12(3) | 01-15 | e2425
Submitted: 2024-01-24
Accepted: 2024-07-01

Modelagem Computacional Multifísica de Reatores Nucleares de Pequeno Porte Através do Acoplamento dos Códigos Serpent e Fluent

Resumo: A pesquisa sobre energia nuclear usando códigos computacionais tem sido amplamente explorada por pesquisadores em engenharia nuclear ao longo dos anos, com ênfase em cálculos neutrônicos e termo-hidráulicos. A necessidade de projetar um modelo de reator que produzisse energia a um custo menor por MWh destacou a importância dos Reatores Modulares de Pequeno Porte (SMR). **Desenvolvimento:** O presente trabalho tem como objetivo implementar e avaliar o acoplamento de dois códigos computacionais, SERPENT e ANSYS FLUENT, na simulação computacional do reator SMR PWR (Reator de Água Pressurizada) da empresa B&W Generation, chamado mPower. **Métodos:** A geometria de um pino do reator mPower foi modelada e as análises neutrônicas do modelo foram realizadas usando o código SERPENT, enquanto as análises termo-hidráulicas foram suportadas pelo código FLUENT. Um algoritmo de acoplamento entre as duas ferramentas de simulação foi construído para automatizar o processo de obtenção das condições operacionais para o funcionamento efetivo do reator. **Resultados:** Este trabalho possibilitou o desenvolvimento de uma ferramenta que realiza o acoplamento entre os fenômenos neutrônicos e termo-hidráulicos do pino do reator mPower, permitindo a modelagem multifísica do reator. **Conclusão:** A simulação multifísica, considerando a interação entre os fenômenos neutrônicos e térmicos, oferece uma visão aprimorada da operação do reator. Ela é suportada pelo acoplamento entre os fenômenos, onde a distribuição de potência no volume produzida pela simulação neutrônica é aplicada na entrada da simulação termo-hidráulica, e a distribuição temperaturas calculada na simulação termo-hidráulica é aplicada a uma nova iteração da simulação neutrônica. Para obter boas estimativas nas grandezas de interesse (distribuição de potência e temperatura), a linguagem Python foi utilizada na implementação de um processo automatizado de acoplamento.

Palavras-chave: SERPENT, FLUENT, mPower, reatores nucleares, acoplamento multifísico, modelagem computacional.

SBPR

1. INTRODUCTION

Due to the global population and economic growth, energy demand increases, exacerbating environmental challenges linked to global warming. Traditional energy sources, based on fossil fuels, contribute to increased greenhouse gas emissions. Therefore, nuclear energy, especially Small Modular Reactors (SMRs), emerges as a sustainable low-carbon alternative. SMRs are advantageous due to their ability to meet local needs, reduce costs, and provide flexibility [1]. They can complement intermittent renewable energy sources, such as solar and wind, by providing a continuous energy supply and maintaining energy security [2]. SMR development is on the rise, boosting global nuclear production with reduced investment. They have diverse applications, including generating electricity, producing heat for industrial processes, and projects such as desalination and hydrogen production.

The U.S. integral Pressurized Water Reactor (iPWR) project leverages past experience with light water reactors (LWR), facilitating their future construction. In recent years, there has been a significant effort to simplify computational tools used in these studies, aiming to simulate reactor behavior in real or hypothetical conditions more efficiently. The thermo-hydraulic and neutronic coupling was studied with the goal of developing code for an Egyptian ETRR-2 reactor for research and simulation of reactivity risks in the reactor [3]. The Computational Fluid Dynamics (CFD) FLUENT, coupled with point kinetics equations, was also used to simulate the risk of loss of coolant flow without emergency shutdown (SCRAM) in the Material Testing Reactor (MTR) research reactor, applied for safety assessment, to determine the stability limits of two-phase flow as a function of reactor initial conditions [4]. In the thermo-hydraulic and neutronic coupling of the CROCUS research reactor, the SERPENT 2 code was used to generate group neutronic parameters that were used in the PARCS code. The neutronic model was then integrated into the TRACE thermo-hydraulic

code for transient analyses [5]. A coupled Monte Carlo-CFD analysis of heat transfer phenomena in a fuel assembly of a supercritical water reactor was also performed, applying a methodology that combines the Monte Carlo code MCNP5 with the CFD software ANSYS FLUENT to simulate heat flow behavior in supercritical water conditions [6].

SMR reactors are the future of clean and safe energy generation. Research involving these types of reactors is important to better understand the dynamics of heat transfer and power generation in the systems. In this context, the studies presented are interesting but need to be more comprehensive by including new SMR designs and considering more general operational conditions. This present work aims at coupling thermo-hydraulic and neutronic aspects for the mPower research reactor, where, for the analysis of neutronic phenomena, the SERPENT-2 software is being utilized, and for the analysis of thermo-hydraulic phenomena, the CFD FLUENT software is being used, in order to validate previous studies conducted with the model in question [7]. The multiphysics coupling offers an improved description of operational conditions.

2. MATERIALS AND METHODS

This work uses the SERPENT code to perform neutron transport calculations, a stochastic approach developed in VTT (*Valtion Teknillinen Tutkimuskeskus*) Technical Research Centre of Finland [8]. SERPENT is a versatile and comprehensive tool for neutronics analysis in nuclear reactors, being able to model three-dimensional geometries. The output data are easily controlled and cover many isotopes of fission products, considering decay chains [7]. Based on the Monte Carlo method, SERPENT configures itself with cross-section libraries and adapts to boundary conditions. The Monte Carlo method, widely applied in various areas such as finance and physics, is a statistical technique that uses random generation to solve complex problems [9]. The method generates a large number of

random values to simulate systems and statistics calculations [10]. Its flexibility allows application to diverse problems supporting simulations with high computational cost. However, it can be computationally intensive and may requires many iterations to obtain results [11]. The estimated error (R) in this method consists of the statistical estimate as the result of the fraction of the estimated mean:

$$R = \frac{S_{\bar{x}}}{\bar{x}}$$

where:

R: statistical results;

S_x: standard deviation;

x: number of samples.

The error is used in creating confidence intervals for the estimated mean. According to the central limit theorem [12], when the number of independent trials (N) is large enough, about 68% of the time, the final result will be within the interval $\bar{x} \pm \bar{x}R$, and 95% of the time, it will be within the interval $\bar{x} \pm 2\bar{x}R$.

Computational Fluid Dynamics, or CFD (Computational Fluid Dynamics), is an approach to studying heat and mass transfer by simulating physical and chemical processes in fluid flows. This involves the analysis of speed, pressure, temperature, and the type of flow (laminar or turbulent), which depends on the Reynolds number. The fundamental equations include the conservation of mass, energy, and momentum, expressed through the continuity equations, energy conservation, and the Navier-Stokes equations. The Navier-Stokes equations are a set of nonlinear partial differential equations that describe the movement of incompressible fluids, relating pressure, velocity, and density. Due to their complexity, these equations cannot be solved analytically. Currently, methods such as finite differences, finite elements and finite volumes [13] allow solving these system equations. In the area of fluid dynamics, the FLUENT package uses these Navier-Stokes equations and the conservation

of mass to analyze dynamic problems of incompressible Newtonian fluids. The Navier-Stokes equations for incompressible fluids are based on linear momentum balance laws. The equations governing the hydrodynamic problem of an incompressible Newtonian fluid include the Navier-Stokes equations and the conservation of mass protection and are described by:

$$\rho \frac{\partial v}{\partial t} + \rho v * \nabla v - \mu \Delta v + \nabla p = f$$

$$\nabla \cdot v = 0$$

coupled with an initial condition for the velocity field and defined boundary conditions, where:

v: fluid velocity;

ϱ: density;

t: time;

μ: fluid dynamic viscosity;

p: pressure;

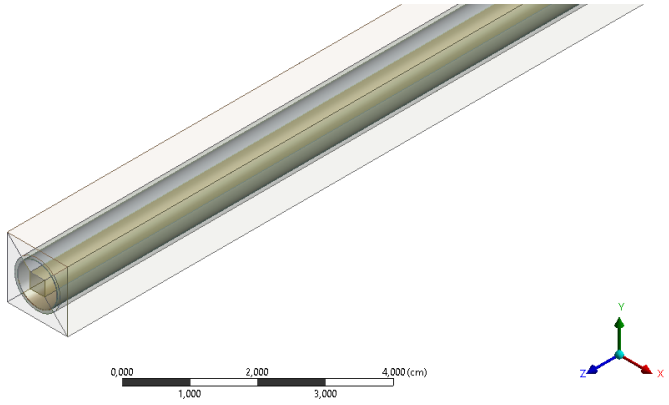
f: external forces acting on the body (such as gravity).

The energy equation derives from the first law of thermodynamics, relating the rate of change of energy to heat and work in a control volume. Work is calculated as the product of surface forces and velocity. Energy flows follow Fourier's law for heat conduction. Dissipation (ψ) represents the energy dissipated due to fluid deformation. The energy of the fluid includes internal, kinetic, and gravitational potential energies [14].

The moment balance equations, mass balance, and energy conservation, together with boundary conditions, make up the mathematical model of fluid dynamics. Numerical resolution is done using the finite volume method in the FLUENT code. To model the

thermo-hydraulic phenomenon observed in the considered reactor, FLUENT software was used to analyze flow, cooling, pressure, and temperature. The geometric model shown in the Figure 1, with the pin representing the fuel rod, helium and zirconium coating was used in FLUENT simulations.

Figure 1: Pin FLUENT geometrical model for mPower reactor.



For neutron analysis, the SERPENT-2 software was used, and through it the geometry of the reactor pin was developed, as shown in Figure 2. The computational domain uses the one-pin model of the mPower reactor; its characteristics appear in Table 1. A simulation input script was developed with the physical and chemical characteristics of the pin, as well as the energy detector to monitor the vertical distribution of energy [7].

The mPower reactor has 69 fuel assemblies arranged in a square lattice, with water as coolant and heat carrier. The thermal power is evenly distributed across each pin, with a total of 530 MW. The heat generation on each pin was calculated as 530 MW / 69 sets / 264 pins, resulting in 31,565.65 W. However, for the study conducted in this work, the highest pin power reported in the mPower reactor was used. According to Betancourt [7] the pin thermal power was 56,318.20 W. Other reported mPower parameters from [7] were also utilized to support this study.

Figure 2: Arrangement of materials and pin geometry of the mPower reactor, computational model for Serpent code.

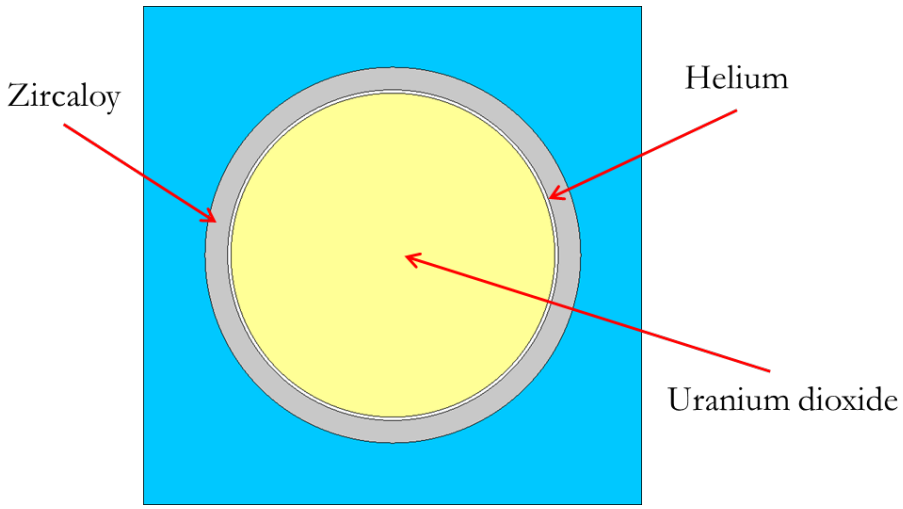


Table 1: Pin data from the mPower reactor fuel assembly used as a geometric simulation model [7].

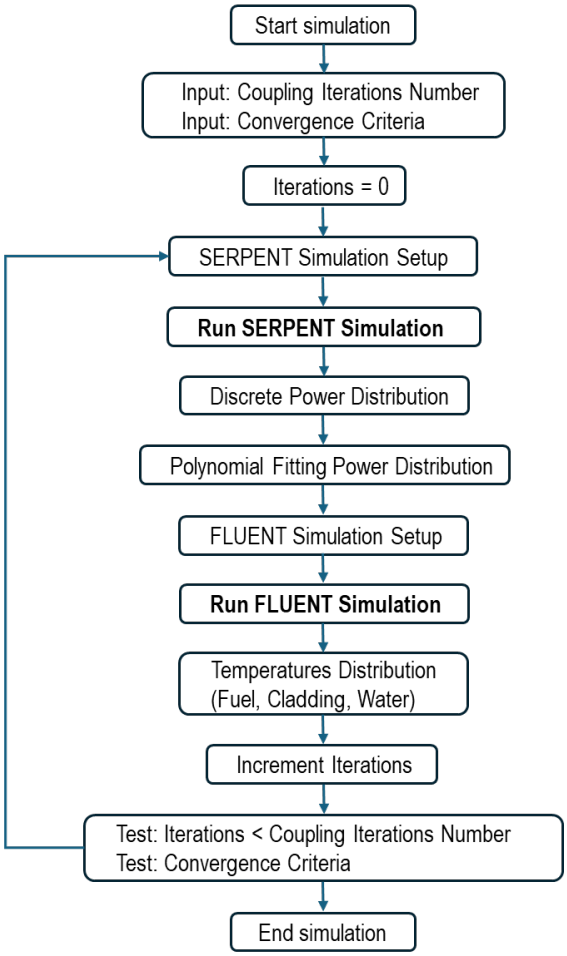
Parameter	Value
Fuel rod radius	0.4096 cm
Inner casing radius	0.418 cm
Outer radius of the casing	0.475 cm
Network step of the elements	1.26 cm
Fuel material	UO2
Coating material	Zircaloy-4
Guide tube inner radius	0.561 cm
Outer radius of the guide tube	0.602 cm
Inner radius of instrumentation tube	0.559 cm
Outer radius of instrumentation tube	0.605 cm
Tube material	Zircaloy-4
Spacing between sets	0.04 cm
Fill gas material	Helium
Pin height	240 cm

3. RESULTS AND DISCUSSIONS

For the integration between neutronic and thermo-hydraulic simulations, we used BotCity [15]., an easy-to-use cloud chatbot platform for creating conversational bots without advanced programming skills. The Tkinter Python library [16] was used to create an intuitive graphical user interface (GUI), allowing the development of custom visual elements and

layouts. These tools and Python programming were used to develop the automated coupling algorithm, as shown in Figure 3.

Figure 3: Coupling procedure flux diagram.



The coupling procedure begins by setting a maximum number of iterations and a convergence criterion. Using the SERPENT model and initial guesses for material temperatures, we run a neutronic simulation. The generated power distribution is then fitted to a sixth-degree polynomial. This polynomial is used as a User Defined Function (UDF) in the FLUENT setup setting the thermal sources inside domain. A thermal simulation is subsequently performed, yielding new temperature distributions. At this point, convergence is checked, resulting in either a feedback loop, which updates the SERPENT setup and

repeats the process, or the termination of the simulation. Upon completion of the coupling process, we obtain robust power and temperature distributions.

In the computational experiments, we set the coupling procedure to run for 10 iterations. After 10 iterations, the relative deviations between power and temperature distributions in subsequent estimates were less than 1%. During the coupling simulations, various relevant quantities were displayed in the graphical interface. For the SERPENT calculations, a polynomial fit for the power distribution was displayed. For example, the polynomial in the first iteration appeared as follows:

$$P(y) = (-0.588z^6 + 3.728z^5 - 5.300z^4 - 6.173z^3 + 4.866z^2 + 20.82z + 19.15)10^7 \quad [W/m3^3]$$

for the FLUENT simulation, the average temperatures in each relevant material (fuel, Zircaloy, and water) are displayed in the interface. After the first iteration, the average temperatures are 804.39 K, 601.35 K, and 578.09 K, respectively. Additionally, after completing the neutronic simulation step, a graphical interface generates a plot of the power distribution to verify its coherence with the physical problem, as shown in Figure 4.

Table 2 shows the changes in the average temperatures of the water, Zircaloy, and UO2 regions. It is clear from Table 2 that the iterated temperatures converge to a region of stability, presenting a small relative deviation between iterations, as shown in Table 3.

Figure 4: Power distribution along the pin in the cladding.

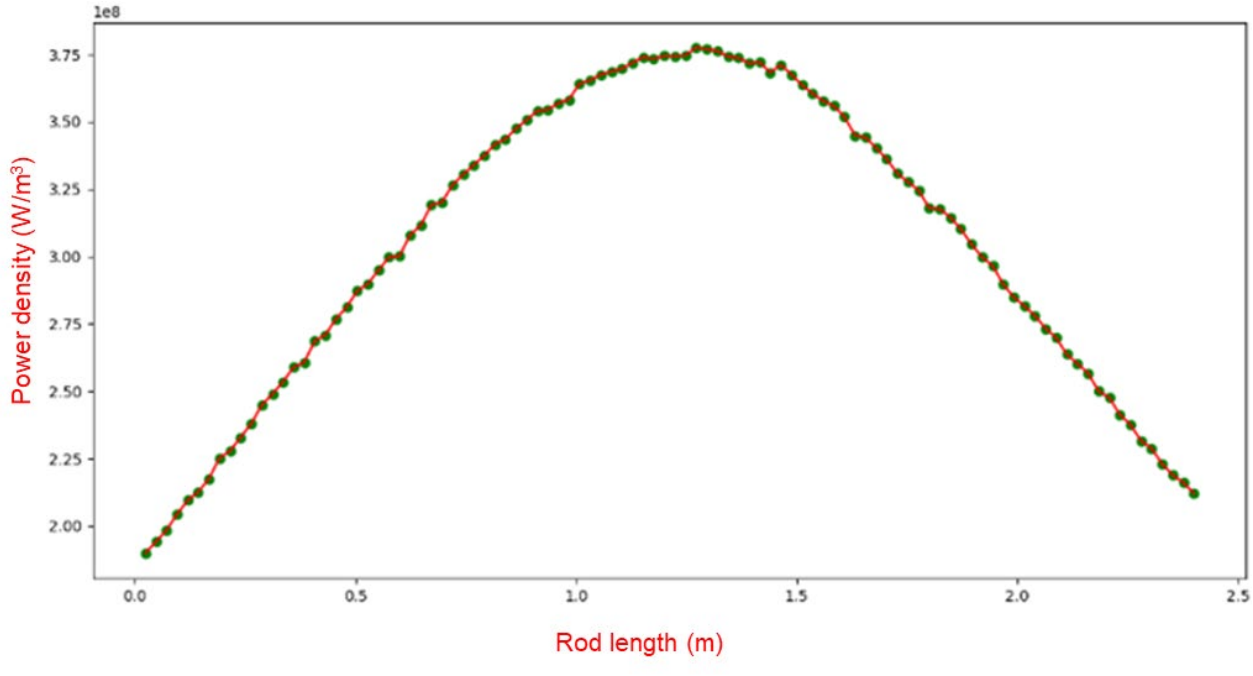


Table 2: Averages temperatures of the material regions along 10 iterations.

ITERATION	WATER TEMP. (K)	ZIRCALOY TEMP. (K)	UO_2 TEMP. (K)
0	580.00	650.00	950.00
1	578.09	601.35	804.39
2	578.12	601.06	801.77
3	578.45	601.91	806.50
4	577.96	601.22	804.28
5	578.07	601.03	801.03
6	578.46	601.70	804.58
7	578.28	601.47	804.04
8	578.19	601.28	803.07
9	578.58	602.04	806.61
10	578.25	601.50	804.46

Table 3: Relative error on the average temperatures in the material regions along 10 iterations.

ITERATION	WATER TEMP. RELATIVE ERROR(%)	ZIRCALOY TEMP. RELATIVE ERROR(%)	UO2 TEMP. RELATIVE ERROR(%)
0	-	-	-
1	0.33	7.48	15.33
2	0.01	0.05	0.33
3	0.06	0.14	0.59
4	0.08	0.11	0.28
5	0.02	0.03	0.40
6	0.07	0.11	0.44
7	0.03	0.04	0.07
8	0.02	0.03	0.12
9	0.07	0.13	0.44
10	0.06	0.09	0.27

Table 3 shows a relative error of below 1%, except for the first iteration with the initial guessed reactor temperatures, which converged throughout the iterations. This behavior suggests that the coupling mechanism is effective, producing convergence of temperatures to a constant value. Compared with the results obtained by Betancourt [7], our results were satisfactory, demonstrating robust behavior during the coupling process.

4. CONCLUSIONS

In view of the above, multiphysics simulations coupling neutronic and thermal phenomena were carried out on the pin of the mPower reactor. The highest power pin in mPower is 56,318.20 W. Both simulations are complementary, allowing for the coupling where the power distribution from the neutronic simulation was applied to the thermo-hydraulic simulation. The resulting temperatures from the thermo-hydraulic simulation were then used in a new iteration of the neutronic simulation.

During the coupling process, after three iterations, a relative deviation of less than 3% was observed in the power distribution, and a relative error of less than 1% was noted in the temperature distribution. These results indicate a high convergence speed for the coupling.

An automated computational algorithm was developed using Python, enabling users to define the number of iterations required to achieve an approximation with a relative error of less than 1%. The graphical interface facilitates easy visualization of the results, including the polynomial fit of power distribution and the average temperatures of the material regions on the pin. This automated closure method can be extended to multiphysics simulations of core and fuel assemblies, not just pins, using relative error as a criterion to determine when to stop the iterative process.

ACKNOWLEDGMENT

This research was partially supported by Bahia State Research Support Foundation (FAPESB, Fundação de Amparo à Pesquisa do Estado da Bahia). Additionally, we appreciate the partial support of Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

FUNDING

The authors would like to thank the Center for Computational Biology and Biotechnology Information Management (NBCGIB) and its coordinators for the availability and use of equipment. They would also like to thank the FAPESB scholarship (Request 524/2021).

CONFLICT OF INTEREST

All authors declare that they have no conflicts of interest.

REFERENCES

[1] Rodrigues, N.; Raeder, F. Assessing the potential of Small Modular Reactors (SMRs) for the nuclear industry. Energy Test, 2022.

[2] Shahsavari, H., Smart, Stable, Reliable. IAEA Bulletin – Nuclear Power and the Clean Energy Transition, vol 61 (3), 2020.

[3] KHATER, H., ABU-EL-MATY, T., EL-MORSHDY, S. E.-D., Thermalhydraulic modeling of reactivity accident in MTR reactors, Annals of Nuclear Energy, v. 34, n. 9, pp. 732-742, 2007.

[4] KHATER, H., ABU-EL-MATY, T., & EL-MORSHDY, S. E.-D., Thermal-hydraulic modeling of reactivity accident in MTR reactors. Annals of Nuclear Energy, 34(9), 732–742, 2015.

[5] RAIS, A., SIEFMAN, D., GIRARDIN, G., HURSIN, M., & PAUTZ, A., Methods and Models for the Coupled Neutronics and Thermal-Hydraulics Analysis of the CROCUS Reactor at EFPL. Science and Technology of Nuclear Installations, 2015, 1–9.

[6] CASTRO, L., FRANÇOIS, J.-L., & GARCÍA, C., Coupled Monte Carlo-CFD analysis of heat transfer phenomena in a supercritical water reactor fuel assembly. Annals of Nuclear Energy, 141, 107312, 2020.

[7] Betancourt, M. C.; Hernandez, C. R. G.; Dominguez, D. S.; Mazaíra, L.; Brayner, C. A.; García, J. A. R.; Iglesias, S. M., Mixed-oxide fuel strategies in an integral pressurized water reactor. Progress in Nuclear Energy, 139, 103844, 2021.

[8] Leppanen, J.; Pusa, M.; Viitanen, T.; Valtavirta.; Kaltiaisenah, T., "The Serpent Monte Carlo code: Status, development and applications in 2013," Annals of Nuclear Energy, vol. 82, pp. 142–150, 2015.

[9] Sobol, I. M. A Primer for the Monte Carlo Method. Journal of the American Statistical Association, 92(440), 1997.

[10] Robert, C. P.; Casella, G. Monte Carlo statistical methods. Springer Science & Business Media. 2010.

[11] Kroese, D. P.; Taimre, T.; Botev, Z. I. Handbook of Monte Carlo methods. John Wiley & Sons. 2014.

[12] Fraley, B. J. MCNPTM – A general Monte Carlo n-particle transport code version 4C. Manual LA–13709–M, Los Alamos, 2000.

[13] Pritchard, P.; Mitchell, J., Fox and McDonald's Introduction to Fluid Mechanics, 9th Edition. Wiley, 2015.

[14] Zingg. D.W., Fundamentals of Computational Fluid Dynamics, NASA Ames Research Center, University of Toronto Institute for Aerospace Studies, Toronto, CN, 1999.

[15] BotCity. Available at: https://pt-br.botcity.dev. Accessed on: 13 Oct. 2022.

[16] Python. Available at : https://docs.python.org/3/library/tkinter.html. Accessed on : 12 Oct. 2022.

LICENSE